# DEVELOPMENT AND VALIDATION OF A REDUCED MF/BIODIESEL MECHANISM FOR DIESEL ENGINE APPLICATION

# by

# Mingrui WEI<sup>a</sup>, Ji GAO<sup>a</sup>, Jinping LIU<sup>b</sup>, and Song LI<sup>b\*</sup>

<sup>a</sup> School of Automotive Engineering, Wuhan University of Technology, Wuhan, China <sup>b</sup> School of Mechanical Engineering, Anyang Institute of Technology, Anyang, China

> Original scientific paper https://doi.org/10.2298/TSCI220509130W

The 2-methylfuran (MF) is widely used as a surrogate fuel for internal combustion engines. However, the chemical kinetics model of MF for engine combustion simulations remains scarce. In this paper, a reduced MF/biodiesel mechanism consisting of 82 species and 226 reactions was proposed and used to simulate the combustion process of MF and biodiesel dual-fuel diesel engine. First, a detailed chemical reaction mechanism of MF was selected and then mechanism reduction methods were used to reduce the detailed mechanism under engine conditions. Second, the reduced MF mechanism was coupled with a biodiesel mechanism to form a four-component chemistry mechanism, consisting of MD, MD9D, n-heptane, and MF. Third, the combined mechanism was optimized by using rate of production analysis and sensitivity analysis. Finally, the proposed four-component mechanism was verified by comparing the calculated values of ignition delay and species concentrations with the experimental values. Meanwhile, a new dual-fuel diesel engine test was carried out, and the experiments were used to evaluate the reliability of the combination mechanism. Overall, the simulated results of the proposed four-component mechanism in this paper are basically consistent with the experimental results.

Key words: 2-methylfuran, biodiesel, reaction mechanism, dual-fuel engine

# Introduction

Since the 21<sup>st</sup> century, in order to overcome the scarcity of fossil fuels, researchers have to find clean renewable fuels which can replace traditional fossil fuels. Among various surrogate fuels, biodiesel and alcohols have aroused great interest as substitutes for automobile fuel. Biodiesel is a monoalkyl ester of long-chain fatty acids extracted from animal fats or vegetable oils [1], which has the key properties of non-toxic, high cetane number, high oxygen content, non-sulfur, high inherent lubricity and biodegradability. These properties make this fuel an ideal substitute for fossil diesel. Alcohols are regarded as substitutes for gasoline or additives for diesel. Ethanol is the most widely studied, but its application is limited because of its low energy density, high production cost, strong volatility and high water solubility [2, 3]. Therefore, many studies have been carried out to find better gasoline substitutes or diesel additives than alcohols.

With the in-depth research on biofuels, MF has attracted more and more attention as a promising renewable fuel for internal combustion engines. The MF can be produced from non-edible biomass [4-6] and the potential of MF as surrogate fuel on engine has been proved

<sup>\*</sup> Corresponding author, e-mail: lisong57528@foxmail.com

[7, 8]. As shown in tab. 1 [9-11], the boiling point of MF is similar with gasoline, and its high octane number makes it suitable as a substitute for gasoline. In addition, MF has several advantages over smaller alcohols. The MF has higher energy density (~29 MJ/L) compared to ethanol (~21 MJ per Litre) and *n*-butanol (~27 MJ per Litre), which is close to gasoline (~32 MJ per Litre) [12].

	Diesel	Biodiesel	Ethanol	Gasoline	MF
Molecular formula	C <sub>12</sub> -C <sub>25</sub>	C <sub>12</sub> -C <sub>24</sub>	C <sub>2</sub> H <sub>5</sub> OH	C <sub>4</sub> -C <sub>12</sub>	C <sub>5</sub> H <sub>6</sub> O
Cetane number	55	52	8	10-15	9
Research octane number	_	_	108	90-99	103
Oxygen content [wt.%]	0	10	34.8	0	19.5
Density at 20 °C [gcm <sup>-3</sup> ]	0.82	0.88	0.79	0.745	0.913
Boiling point [°C]	180-360	262-359	78.4	27-225	64.7
Viscosity at 20 °C [mm <sup>2</sup> s <sup>-1</sup> ]	4.8	8.9	1.08	0.4-0.8	-
Low heating value [MJkg-1]	42.8	38.0	26.8	42.7	31.2
Latent heating at 25 °C [kJkg <sup>-1</sup> ]	270	320	904	380-500	358
Auto-ignition temperature [°C]	210	363	434	420	450
Stoichiometric A/F ratio	14.3	12.5	9.02	14.7	10.05

Table 1. Properties of diesel, biodiesel, ethanol, gasoline and MF [9-11]

The applicability of MF fuel as gasoline surrogate fuel or diesel additives in internal combustion engines has been experimentally evaluated in many studies. Wang et al. [7] investigated the performance of a direct-injection spark-ignition (DISI) engine fueled with MF, ethanol, gasoline and 2,5-dimethylfuran (DMF). The experiments showed that MF produces a higher indicated thermal efficiency than gasoline and DMF, and the emissions of aldehydes of MF are lower than those of gasoline and ethanol. Feng et al. [13] studied the combustion and emissions performance of MF/gasoline mixtures on a spark-ignition (SI) engine. The results showed that compared with gasoline, MF has better knock suppression ability. Meanwhile, the combustion duration of MF/gasoline mixtures was shorter, and the maximum in-cylinder pressure and average temperature were higher than those of gasoline. The emissions of HC and CO were significantly reduced. Sivasubramanian et al. [14] conducted an experimental study on the effects of MF addition on engine combustion performance and emissions performance in a four-stroke multi-point fuel injection (MPFI) SI engine. The experimental results showed that with the increase of blend percentage, the ignition delay time was reduced, the emissions of CO and HC decrease, while braking thermal efficiency (BTE) and  $NO_x$  emissions increase. Xiao et al. [15-17] studied the performance of MF/diesel and MF/biodiesel blends in a direct-injection compression-ignition (DICI) engine. They found that MF/diesel mixtures have longer ignition delays, shorter combustion duration and higher BTE. Meanwhile, MF addition could effectively reduce the emissions of HC, CO and soot, while the emissions of NO, are increased. Liu et al. [18] investigated the performance of MF in a DISI engine and found that when considering combustion phasing and knock limit, the spark timing range of MF is larger than that of gasoline. Compared with gasoline and ethanol, MF has more robustness to lean combustion.

The chemical kinetics mechanism of MF has also been studied by several researchers. Somers *et al.* [19] proposed a detailed DMF mechanism with 545 species and 2768 reactions, which includes the chemistry mechanism of MF. The prediction ability of detailed mechanism was widely evaluated by comparing with the experimental measurements, including ignition de-

1466

lays at pressure of 1, 20, and 80 bar, equivalence ratios (ER) of 0.5-2.0 and temperature of 820-1800 K, jet-stirred reactor (JSR) species mole fraction profiles at temperatures of 770-1220 K, 10.0 atm, and ER of 0.5-2.0, and laminar burning velocities at atmospheric pressure, temperatures of gas at 298 and 358 K and ER of 0.6-1.6. Later, Somers *et al.* [20] modified the reaction rates of MF by statistical rate theory, quantum chemical calculation and chemical kinetic model. Somers *et al.* [21] also proposed a chemical kinetic model for MF oxidation consisting of 391 species and 2059 reactions. The ignition delays predicted by this mechanism were evaluated by experimental results of shock tube ignition delays at pressure of 1 atm, temperatures of 1200-1800 K and ER of 0.5-2.0, and laminar flame velocities at temperatures from 298 to 398 K, pressure of 1 atm and ER of 0.55-1.65. They found that the developed mechanism could accurately predict the experimental measurements. Tran *et al.* [12] developed a detailed chemical kinetic model for MF oxidation, which is composed of 305 species and 1472 reactions. It was verified by comparing the predicted species mole profiles with the experimental data in MF/O<sub>2</sub>/Ar at pressures of 20 and 40 mbar and ER of 1.0 and 1.7.

From the aforementioned works, the reduced MF/biodiesel mechanism applicable to Diesel engine simulation has not been reported. This paper presents a reduced four components mechanism, consisting of MF, MD, MD9D and *n*-heptane, for simulate MF/biodiesel dual-fuel engine. The performance of this mechanism was verified by comparing the simulations and the experimental measurements of ignition delays in shock tubes and species mole fractions in laminar premixed flames. In addition, the combustion performances of biodiesel and MF was studied on a dual-fuel diesel engine, and the reduced mechanism was further evaluated by comparing with the experimental results.

# Kinetic model construction

# Base biodiesel mechanism

The biodiesel mechanism with 69 species and 192 reactions developed by Brakora *et al.* [22] was adopted as base mechanism, in which a mixture of 25% methyl decanoate (MD), 25% methyl-9-decanoate (MD9D), and 50% *n*-heptane were used as biodiesel surrogate fuels, where MD and MD9D were, respectively used as the surrogates for saturated and unsaturated species in actual biodiesel, and *n*-heptane was used to improve ignition behavior. Then they investigated experiments to prove the accuracy of the mechanism. The results showed that, at low speed, high load, the performance and NO<sub>x</sub> formation of the experiment are accurately predicted by the mechanism and the kinetic model can also well-predicted the consumption of HC, CO, NO<sub>x</sub>, and fuel at high speed and low load.

# The reduced MF mechanism

A detailed mechanism of MF oxidation proposed by Tran *et al.* [12], consisting of 305 species and 1472 reactions, was selected as the initial mechanism. First, the direct relation graph error propagation (DRGEP) method was employed to systematically remove the decoupled species and unrelated reactions at a chosen error limit of 30% in the first reduction process. The reduction process of the detailed MF mechanism was carried out at the pressure of 1-10 atm, temperature of 800-1600 K within the ER of 0.5-2.0. In each reduction step, the performance of the ignition delay of generated reduction mechanism is compared with the startup mechanism to ensure that it maintains an acceptable predictive ability. Second, manual reductions were carried out by using the methods of rate of production analysis (ROPA) and sensitivity analysis (SA). Third, isomer lumping method was used to further reduce the number of reactions. Finally, a reduced MF mechanism consisting of 42 species and 148 reactions was formed.



Figure 1. Reaction path analysis carried out at 20% fuel consumption under shock tube conditions at T = 1300 K, 40 bar for stoichiometric MF/N/O<sub>2</sub> mixtures

#### The combined mechanism

A reaction path analysis of the reduced MF mechanism and simulation time corresponding to around 20% fuel conversion was conducted in a homogeneous batch reactor for an ignition process of stoichiometric MF/O<sub>2</sub>/ Ar mixtures at 40 bar pressure and 1300 K. As shown in fig. 1, there are two major consumption paths of MF. The MF is primarily consumed (~70.2%) by H-abstractions from the methyl group forming the furylCH<sub>2</sub> radical. Then about 63.8% furyICH2 radicals were isomerized to form OCHCHCHCCH2 radical, and then OCCHCHCHCH2 radical were formed. OCCHCHCHCH2 decomposed into the C4H5 radical and CO by  $\alpha$ -cleavage of the C-C bond and about 36.2 % furyICH<sub>2</sub> yields furyICH<sub>2</sub>O and then generates furyl-2. A second important path of consumption of MF is to yield furan by ipso-addition. As for the decomposition of furan, about 68.9% of furan yields C2H3CHO by OH-addition at the C = C double bond and further cleavage to C<sub>2</sub>H<sub>2</sub>. About 31.1 % of furan generates furyl-2 by H-abstractions at C<sub>2</sub> position. furyl-2 further cleavage to CH<sub>2</sub>CHCO and CHCHCO.

The reduced MF mechanism is coupled with Brakora *et al.* [22] biodiesel mechanism, and the repetitive reactions in the base mechanism were remained. After the merger process, a combined mechanism with 82 species and 226 reactions was obtained. Initial shock tubes simulation results showed that the calculated value of the ignition delay by this combined mechanism has a large error with the experimental value, so it is necessary to optimize the combined mechanism.

Based on the ROPA and SA methods, several reactions were adjusted in this base mechanism to improve its prediction of ignition delays. The following reaction (R1) is most sensitive to the ignition delays of *n*-heptane and the pre-exponential factor was adjusted from  $1.355 \cdot 10^{10}$  to  $1.355 \cdot 10^{13}$ . The reaction with high sensitivity to MD9D ignition delay is (R2), and the pre-exponential factor of (R2) was adjusted from  $2.5 \cdot 10^{10}$  to  $2.5 \cdot 10^{8}$ .

$$NC_7H_{16} + OH = C_7H_{15} - 2 + H_2O$$
 (R1)

$$MF_5O_2 = MF_5OOH_3J$$
(R2)

In addition, it was found that the two reactions of (R3) and (R4) are the most sensitive to MF ignition delay times in the combined mechanism. Thus the reaction rate coefficients of (R3) was adjusted from  $1.0 \cdot 10^{14}$  to  $1.0 \cdot 10^{13}$  in this study, while (R4) was adjusted from  $4.5 \cdot 10^{16}$  to  $4.5 \cdot 10^{18}$  to match the experimental ignition delays.

$$C_4H_5 = C_2H_2 + C_2H_3$$
(R3)

$$C_4H_5 + O_2 = HCO + C_2H_3CHO$$
(R4)

Finally, a reduced MD/MD9D/*n*-heptane/MF mechanism which contains 82 species and 226 reactions was formed.

# **Mechanism validation**

Ignition delays, premixed flame species mole fraction, dual-engine in-cylinder pressure predicted by the proposed MD/MD9D/*n*-heptane/MF mechanism were compared and verified with the measurement results in this section.

#### Ignition delay times

Figure 2 shows the comparison of the predicted ignition delays of *n*-heptane of the reduced mechanism with measurements of Ciezki *et al.* [23] and Hartmann *et al.* [24] under the ER of 1.0 and 2.0, and initial pressures of  $13.5 \sim 42$  bar. As shown in fig. 2, the proposed mechanism can well-predict the experimental shock tube data of *n*-heptane, especially the negative temperature coefficient (NTC) phenomenon could be well captured.



Figure 2. Measured [23, 24] (symbols) and predicted (lines) ignition delays of *n*-heptane

Wang *et al.* [25, 26] studied the experiment of the ignition delays of MD/air blends at pressures of 16 and 21 bar, temperatures of 650-1350 K within the ER of 0.5, 1.0, and 1.5. Figure 3 shows the comparison between ignition delays predictions and the experimental data of MD. It could be seen that the reduced mechanism can accurately predict the ignition delays of MD. Decrease of the ignition delays with increase of ER could be well captured, indicating that the reduced mechanism can ensure the accuracy of the prediction of MD ignition delays data.

Ignition delays of MD9D/air mixtures under the pressure of 20 bar within the temperature from 650-1350 K and ER of 0.5-1.5 were measured by Wang *et al.* [26]. In fig. 4, the predicted ignition delays by reduced mechanism was compared with the experimental data. It can be seen that the reduced mechanism satisfactorily predict the measurements, and the phenomenon that ignition delay times are decreased with the increase of ER was observed. In general, the proposed mechanism can reasonably sufficient to simulate the ignition delays of MD9D.

Figure 5 compares of the ignition delays of stoichiometric MF simulated by the proposed mechanism with the experimental data of Eldeeb *et al.* [27] at the pressures of 2 atm, 5 atm,



and 10 atm within the temperature range from 977-1570 K. As seen, the ignition delays increase with the decrease of pressure could be reasonably captured by the reduced mechanism under studied temperature range, which indicates the reduced mechanism can accurately reproduce the measurements under different initial pressure.

#### Premixed flame species profiles

Seidel *et al.* [28] experimentally investigated premixed stoichiometric flame of *n*-heptane/O<sub>2</sub>/Ar mixtures at pressure of 0.04 bar. Figure 6 compared the species mole fraction profiles of experimental values and the predicted values of the reduced mechanism in *n*-heptane premixed flame. For comparison, the simulated results of Brakora *at al.* [22] mechanism were also included.

As shown in figs. 6(a)-6(c), the reduced mechanism accurately predicts the experimental measurements of the concentrations of *n*-heptane, O<sub>2</sub>, Ar, and CO, but there are some discrepancies in CO<sub>2</sub>, H<sub>2</sub>O and H<sub>2</sub> concentrations. At the lower height of above burner (HAB), the simulations of H<sub>2</sub> and CO<sub>2</sub> are lower than the experimental measurements, while the simulation of H<sub>2</sub>O are higher than the measurements. With the consumption of *n*-heptane, the simulated concentration values of CO<sub>2</sub>, H<sub>2</sub>O, and H<sub>2</sub> are gradually close to the experimental

Wei, M., et al.: Development and Validation of a Reduced MF/Biodiesel ... THERMAL SCIENCE: Year 2023, Vol. 27, No. 2B, pp. 1465-1477



Figure 6. Measured [28] (symbols) and predicted (lines) species profiles in premixed *n*-heptane flame; solid lines: the proposed mechanism, dashed lines: the Brakora *et al.* [22] mechanism

data. In addition, although the reduced mechanism can accurately predict the concentration of major species, but the difference between simulations and experiments of intermediates is obvious, as shown in figs. 6(e)-6(g). Indeed, although the simulated intermediates by the proposed mechanism is different from the measurements, but the profile shapes of the simulated intermediate species are consistent with the experimental measurements. It is noting that the experimental measurements of H<sub>2</sub>O, CO<sub>2</sub> and intermediates are also not well simulated by the Brakora *et al.* [22] mechanism.

Figure 7 compares the experimental measurements [29] and predicted data of species mole fraction profiles in stoichiometric premixed MD flame at atmospheric pressure. Also, the



Figure 7. Measured [29] (symbols) and predicted (lines) species profiles in premixed MD flame; solid lines: the proposed mechanism, dashed lines: the Brakora *et al.* [22] mechanism

simulation results of Brakora *et al.* [22] mechanism were included. As shown in figs. 7(a) and 7(b), the reduced mechanism accurately predict the concentrations of MD,  $O_2$ , and  $H_2O$ , but there are error in the concentrations of CO and  $CO_2$ . The concentration of CO is higher than the experimental results at the lower HAB, while the simulation of  $CO_2$  is lower than the experimental results. Then with the consumption of  $O_2$  and MD, the simulations of  $CO_2$  and  $CO_2$  are gradually close to the experimental results. As for the mole fraction of intermediates, fig. 7(c) showed that the simulations of  $C_2H_2$  by the reduced mechanism are in excellent agreement with measurements.

Figure 8 compares the simulations of species mole fraction profiles in stoichiometric MD9D/air mixtures premixed flame at atmospheric pressure between the proposed mechanism and Brakora *et al.* [22] mechanism. It was observed that the calculated values of the two mechanisms are in reasonable agreement, indicating that the calculated ability of the MD9D sub-mechanism in Brakora *et al.* [22] mechanism has been well preserved.



Brakora *et al.* [22] mechanism (symbols) in premixed MD9D flame

Tran *et al.* [12] studied the premixed MF flames for ER of 1.0 and 1.7 at pressures of 0.02 bar and 0.04 bar. Figure 9 compares the measurements and simulations of major species mole fraction in premixed MF flames. Also, the simulations of Tran *et al.* [12] mechanism are included. It is observed from fig. 9, the simulated results of MF,  $O_2$ , Ar, and  $H_2$  in premixed stoichiometric flame are consistent with experimental data, but some error between the simulations and experimental data for  $H_2O$ ,  $CO_2$ , and CO has been found. As seen, the simulations of  $H_2O$  and  $CO_2$  are lower than the experimental results and the simulation of CO is higher than the experimental data. In fuel-rich flame, the simulations of MF,  $O_2$ , Ar,  $H_2$ , CO are consistent with

experimental results, but the simulations of  $H_2O$  and  $CO_2$  are lower than the measurements. It is worth noting that the simulated results of  $H_2O$  and  $CO_2$  of Tran *et al.* [12] mechanism are also lower than the measurements.



Figure 9. Measured [12] (symbols) and predicted (lines) species profiles in premixed MF flames; solid lines: the proposed mechanism, dashed lines: the Tran *et al.* [12] mechanism

# Dual-fuel engine combustion validation

To further validate the proposed reduced mechanism of MF/biodiesel, a new dual-fuel diesel engine experiment was conducted in a single-cylinder four-stroke Diesel engine. A detailed description of experimental set-up can be found in [30, 31]. Figure 10 depicts the schematic diagram of the experimental device. Engine specifications and experimental conditions could be found in tabs. 2 and 3. During the experiments, biodiesel was fed into cylinder by a common rail high pressure direct injector, and injection timing was set at -20 ° CA aTDC. The MF fuel was fed into to intake port by a low pressure injector which was installed at intake port, and injection timing was set at -300 °CA aTDC. Keeping the total energy of fuel supplied to engine for each cycle as constant (620.25 J), under the reactivity change compression ignition (RCCI) combustion mode, the premixed ratios of MF/biodiesel dual-fuel was applied as 0%, 40%, and 60% (referred to as D0, D40, and D60) over the energy amount. The multi-dimensional engine simulation was carried out by using the CONVERGE CFD code [32], and the proposed mechanism was imported into the *reaction mechanism* module of CONVERGE as input file. Table 4 shows the physical models selections in the simulation. Figure 11 shows the geometry of the test engine, and simulation range was from -155 °CA aTDC to 155 °CA aTDC.



Figure 10. Schematic of experimental set-up

1	Table 2. Engine specifications				
	Parameter	Value			
	Number of valves	1			
	Bore	96 mm			
	Stroke	115 mm			
	Connecting rod length	210 mm			
	Piston type	flat			
	Intake valve close timing	–155 °CA aTDC			
	Exhaust valve open timing	155 °CA aTDC			

Direct fuel injector

Port fuel injector



Figure 11. Engine sector geometry

Table	3.	Engine	operating	conditions
14010	••	Linginie	operating	contaitions

Parameter	Value
Engine speed	1000 rpm
Intake air temperature	328 K
Intake air pressure	1.07 bar
Direct injection strategy	Single injection
Direct injection timing	–20 °CA aTDC
Port fuel injection timing	-300 °CA aTDC
EGR ratio	0%

Table 4. Computational mouths used in the CI D simulations	Table 4. (	Computational	models used	in the CFD	simulations
--	------------	---------------	-------------	------------	-------------

Bosch, 9 holes, 60 MPa

fuel injection pressure Delphi, 0.5 MPa fuel

injection pressure

Description	Models
Turbulence	RNG <i>k</i> -ε model [33]
Combustion	SAGE model [34]
Turbulent dispersion	O'Rourke model [35]
Droplet collision	NTC collision model [36]
Spray-wall interaction	Wall film model
Spray breakup	KH-RT model [37, 38]
Evaporation	Frossling model [39]
Wall heat transfer	Han and Reitz model [40]

As shown in fig. 12 showed the simulated value of in-cylinder pressure by proposed mechanism was compared with the experimental measurements. The simulations of in-cylinder pressure are in good agreement with the experiments in three simulated conditions, but there are error in the peak of in-cylinder pressure. As shown in figs. 12(a) and 12(b), the simulations of reduced mechanism of combustion duration is longer than the experiments. The slight discrepancies between simulations and experiments may be due to there was no reasonable consideration

on the effect of turbulence on chemical kinetics in the prediction. In addition, there may be some errors of the fuel injection rules between the simulation and experiments. In general, the reduced mechanism could be used to predict the combustion process of MF/biodiesel dual-fuel engine.



## Conclusion

In this work, a reduced MF/biodiesel dual-fuel mechanism with 82 species and 226 reactions was proposed for diesel engine applications. Firstly, the detailed MF mechanism of Tran et al. [12] was selected as the initial mechanism and then the mechanism was reduced by using DRGEP method. Subsequently, ROPA, SA and isomer lumping methods were used to further lessen the number of reactions of the obtained reduced MF mechanism, and a reduced MF mechanism composed of 42 species and 148 reactions was formed. Then the reduced MF mechanism was coupled with the biodisel mechanism of Brakora et al. [22] to form a four-component (MF/MD/MD9D/n-heptane) reaction mechanism. Finally, a MF/biodisel dual-fuel mechanism with 82 species and 226 reactions was obtained by optimizing the reaction rate coefficients in selected reactions. After that, simulations of the new reduced dual-fuel mechanism were compared with the existing experimental measurements, and the results showed that the reduced mechanism can give a good prediction of ignition delays and premixed flame species concentration. In addition, dual-fuel Diesel engine experiments were carried out, and the reduced mechanism was evaluated using corresponding data. It was proven that the proposed mechanism can reasonably capture the experimental in-cylinder pressure. In conclusion, this new MF/biodiesel mechanism could be used to calculate the combustion characteristics of engine fueled with MF and biodiesel.

### Acknowledgment

This research was sponsored by the Key Scientific Research Projects of Colleges and Universities in Henan Province (21B470002), Science and Technology Development Project of Anyang city (2021C01GX006) and Doctoral Start-up Funding of Anyang Institute of Technology (BSJ2019006).

#### Nomenclature

# convine

Acronyms	MD	– methyl decanoate
BTE– braking thermal efficiencyDMF– 2,5-dimethylfuranDICI– direct-injection compression-ignitionDISI– direct-injection spark-ignitionDRGEP– direct relation graph error propagationER– equivalence ratiosHAB– height of above burner, [mm]JSR– jet-stirred reactor	MD9D MF MPFI NTC RCCI ROPA SA SI	<ul> <li>methyl-9-decanoate</li> <li>2-methylfuran</li> <li>multi-point fuel injection</li> <li>negative temperature coefficient</li> <li>reactivity charge compression ignition</li> <li>rate of production analysis</li> <li>sensitivity analysis</li> <li>spark-ignition</li> </ul>
References		

- Venkanna, B. K., Reddy, C. V., Biodiesel Production and Optimization from Calophyllum Inophyllum [1] Linn Oil (Honne Oil)-a Three-Stage Method, Bioresource Technology, 100 (2009), 21, pp. 5122-5125
- Wang H., et al., Development of an n-Heptane-n-Butanol-PAH Mechanism and Its Application for Com-[2] bustion and Soot Prediction, Combustion and Flame, 160 (2013), 3, pp. 504-519
- [3] Vijay Kumar, M., et al., Experimental Investigation of the Combustion Characteristics of Mahua Oil Biodiesel-Diesel Blend Using a DI Diesel Engine Modified with EGR and Nozzle Hole Orifice Diameter, Biofuel Research Journal, 5 (2018), 3, pp. 863-871
- [4] Román-Leshkov Y., et al., Production of Dimethylfuran for Liquid Fuels from Biomass-Derived Carbohydrates, Nature, 447 (2007), June, pp. 982-985
- Tran L. S., et al., Progress in Detailed Kinetic Modelling of the Combustion of Oxygenated Components [5] of Biofuels, Energy, 43 (2012), 1, pp. 4-18
- [6] Lange J., et al., Furfural A Promising Platform for Lignocellulosic Biofuels, ChemSusChem, 5 (2012), 1, pp. 150-166
- [7] Wang, C., et al., Combustion Characteristics and Emissions of 2-Methylfuran Compared to 2,5-Dimethylfuran, Gasoline and Ethanol in a DISI Engine, Fuel, 103 (2013), Jan., pp. 200-211
- Thewes, M., et al., Analysis of the Impact of 2-Methylfuran on Mixture Formation and Combustion in a [8] Direct-Injection Spark-Ignition Engine, Energy and Fuels, 25 (2011), 12, pp. 5549-5561
- [9] Zheng, Z., et al., Experimental Study on the Combustion and Emissions Fueling Biodiesel/n-Butanol, Biodiesel/Ethanol and Biodiesel/2,5-Dimethylfuran on a Diesel Engine, Energy, 115 (2016), Nov., pp. 539-549
- [10] Liu, X., et al., Development of a Reduced Toluene Reference Fuel (TRF)-2,5-Dimethylfuran-Polycyclic Aromatic Hydrocarbon (PAH) Mechanism for Engine Applications, Combustion and Flame, 165 (2016), Mar., pp. 453-465
- [11] Alexandrino, K., Comprehensive Review of the Impact of 2,5-DDimethylfuran and 2-Methylfuran on Soot Emissions: Experiments in Diesel Engines and at Laboratory-Scale, Energy and Fuels, 34 (2020), 6, pp. 6598-6623
- [12] Tran, L. S., et al., Combustion Chemistry and Flame Structure of Furan Group Biofuels Using Molecular-Beam Mass Spectrometry and Gas Chromatography - Part II: 2-Methylfuran, Combustion and Flame, 161 (2014), 3, pp. 780-797
- [13] Feng, D., et al., Engine Combustion and Emissions Characteristics of 2-Methylfuran and Gasoline Blend Fuels, Transactions of Csice, 32 (2014), 4, pp. 340-344
- [14] Sivasubramanian H., Effect of Ignition Delay (ID) on Performance, Emission and Combustion Characteristics of 2-Methyl Furan-Unleaded Gasoline Blends in a MPFI SI Engine, Alexandria Engineering Journal, 57 (2018), 1, pp. 499-507
- [15] Xiao H., et al., Combustion Performance and Emissions of 2-Methylfuran Diesel Blends in a Diesel Engine, Fuel, 175 (2016), July, pp. 157-163

## 1476

Wei, M., et al.: Development and Validation of a Reduced MF/Biodiesel ... THERMAL SCIENCE: Year 2023, Vol. 27, No. 2B, pp. 1465-1477

- [16] Xiao, H., et al., Effects of Pilot Injection on Combustion and Emissions Characteristics Using 2-Methyl-Furan/Diesel Blends in a Diesel Engine, *Thermal Science*, 24 (2020), 1, pp. 1-11
- [17] Xiao, H., et al., Combustion Performance and Pollutant Emissions Analysis of a Diesel Engine Fueled with Biodiesel and Its Blend with 2-Methylfuran, Fuel, 237 (2019), Feb., pp. 1050-1056
- [18] Liu, H., et al., Combustion Characteristics and Engine Performance of 2-Methylfuran Compared to Gasoline and Ethanol in a Direct Injection Spark Ignition Engine, Fuel, 299 (2021), 120825
- [19] Somers, K. P., et al., A Comprehensive Experimental and Detailed Chemical Kinetic Modelling Study of 2,5-Dimethylfuran Pyrolysis and Oxidation, *Combust and Flame*, 160 (2013), 11, pp. 2291-2318
- [20] Somers, K. P., et al., The Pyrolysis of 2-Methylfuran: A Quantum Chemical, Statistical Rate Theory and Kinetic Modelling Study, Physical Chemistry Chemical Physics, 16 (2014), 11, pp. 5349-5367
- [21] Somers, K. P., et al., A High Temperature and Atmospheric Pressure Experimental and Detailed Chemical Kinetic Modelling Study of 2-Methyl Furan Oxidation, *Proceedings of the Combustion Institute*, 34 (2013), 1, pp. 225-232
- [22] Brakora, J. L., et al., Combustion Model for Biodiesel-Fueled Engine Simulations Using Realistic Chemistry and Physical Properties, SAE International Journal of Engines, 4 (2011), 1, pp. 931-947
- [23] Ciezki, H. K., Adomeit G., Shock-Tube Investigation of Self-Ignition of n-Heptane-Air Mixtures under Engine Relevant Conditions, *Combustion and Flame*, 93 (1993), 4, pp. 421-433
- [24] Hartmann, M., et al., Auto-Ignition of Toluene-Doped n-Heptane and Iso-Octane/Air Mixtures: High-Pressure Shock-Tube Experiments and Kinetics Modelling, Combustion and Flame, 158 (2011), 1, pp. 172-178
- [25] Wang, W., Oehlschlaeger, M.A., A Shock Tube Study of Methyl Decanoate Autoignition at Elevated Pressures, *Combustion and Flame*, 159 (2012), 2, pp. 476-481
- [26] Wang, W., et al., Comparative Study of the Autoignition of Methyl Decenoates, Unsaturated Biodiesel Fuel Surrogates, Energy and Fuels, 27 (2013), 9, pp. 5527-5532
- [27] Eldeeb, M. A., Akih-Kumgeh, B., Reactivity Trends in Furan and Alkyl Furan Combustion, *Energy and Fuels*, 28 (2014), 10, pp. 6618-6626
- [28] Seidel, L., et al., Comprehensive Kinetic Modelling and Experimental Study of a Fuel-Rich, Premixed n-Heptane Flame, Combustion and Flame, 162 (2015), 5, pp. 2045-2058
- [29] Gerasimov, I. E., et al., Experimental and Numerical Study of the Structure of a Premixed Methyl Decanoate/Oxygen/Argon Flame, Combustion Explosion and Shock Waves, 51 (2015), 3, pp. 285-292
- [30] Wei, M., et al., Effects of Injection Timing on Combustion and Emissions in a Diesel Engine Fueled with 2,5-Dimethylfuran-Diesel Blends, Fuel, 192 (2017), Mar., pp. 208-217
- [31] Li, S., et al., Effects of Fuel Properties on Combustion and Pollutant Emissions of a Low Temperature Combustion Mode Diesel Engine, Fuel, 267 (2020), 117123
- [32] Senecal, P., et al., CONVERGE (Version 2.4) Manual, Convergent Science Inc., Madison, Wis., USA, 2018
- [33] Han, Z. Y., Reitz, R. D., Turbulence Modelling of Internal Combustion Engines Using RNG k-ε Models, Combustion Science and Technology, 106 (1995), 4-6, pp. 267-295
- [34] Babajimopoulos, A., et al., A Fully Coupled Computational Fluid Dynamics and Multi-Zone Model with Detailed Chemical Kinetics for the Simulation of Premixed Charge Compression Ignition Engines, International Journal of Engine Research, 6 (2005), 5, pp. 497-512
- [35] Amsden, A. A., et al., The KIVA-2: A Computer Program for Chemically Reactive Flows with Sprays, Nasa Sti/recon Technical Report N, NASA, Washington DC, 1989
- [36] Schmidt, D. P., Rutland, C. J., A New Droplet Collision Algorithm, Journal of Computational Physics, 164 (2000), 1, pp. 62-80
- [37] Reitz, R. D., Diwakar, R., Structure of High-Pressure Fuel Sprays, SAE Technical Paper, 870598, 1987
- [38] Reitz R,D, Diwakar R., Effect of Drop Breakup on Fuel Sprays, SAE Technical Paper, 860469, 1986
- [39] Amsden, A. A., The KIVA-3V, Release 2: Improvement to KIVA3V, Los Alamos National Laboratory Report LA-UR-99-915, Los Alamos, Cal., USA, 1999
- [40] Han, Z. Y., Reitz, R. D., A Temperature Wall Function Formulation for Variable-Density Turbulent Flows with Application Engine Convective Heat Transfer Modelling, *International Journal of Heat and Mass Transfer*, 40 (1997), 3, pp. 613-625

Paper submitted: May 9, 2022 Paper revised: June 8, 2022 Paper accepted: July 4, 2022 © 2023 Society of Thermal Engineers of Serbia Published by the Vinča Institute of Nuclear Sciences, Belgrade, Serbia. This is an open access article distributed under the CC BY-NC-ND 4.0 terms and conditions